



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2022 – 08:03 AM EDT

PDB ID : 7U1D  
Title : Crystal structure of arabidopsis thaliana acetohydroxyacid synthase P197T mutant in complex with chlorimuron-ethyl  
Authors : Guddat, L.W.; Cheng, Y.  
Deposited on : 2022-02-21  
Resolution : 3.11 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.28.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.28.1

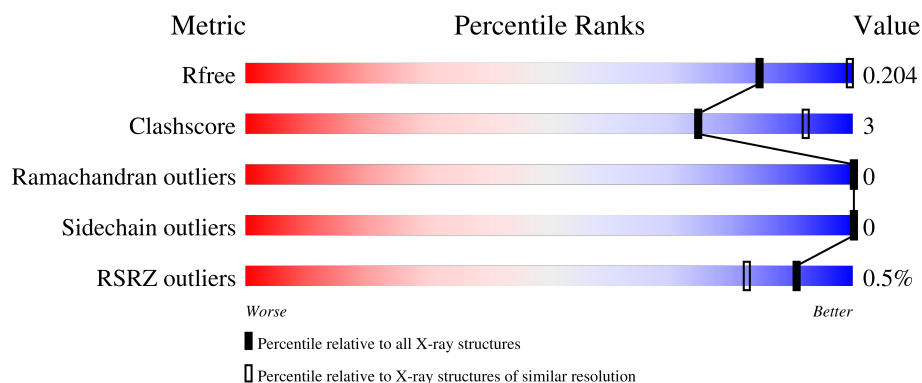
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	582	<div> <div></div> <div>91%</div> <div>9%</div> </div>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 4604 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Acetolactate synthase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	1	0
			4468	2833	770	840	25			

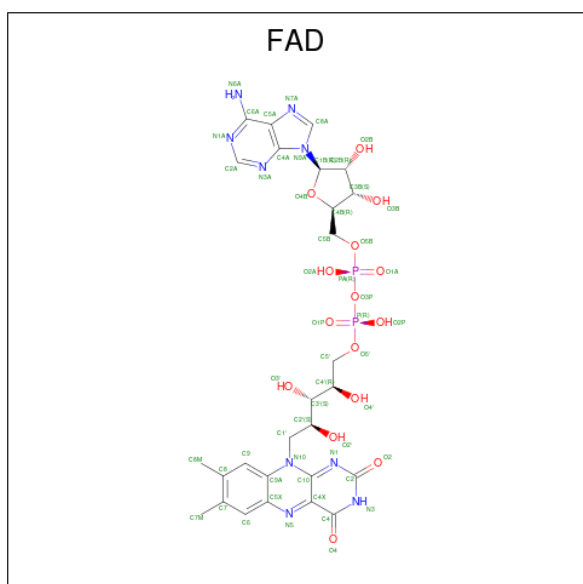
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197	THR	PRO	engineered mutation	UNP P17597

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

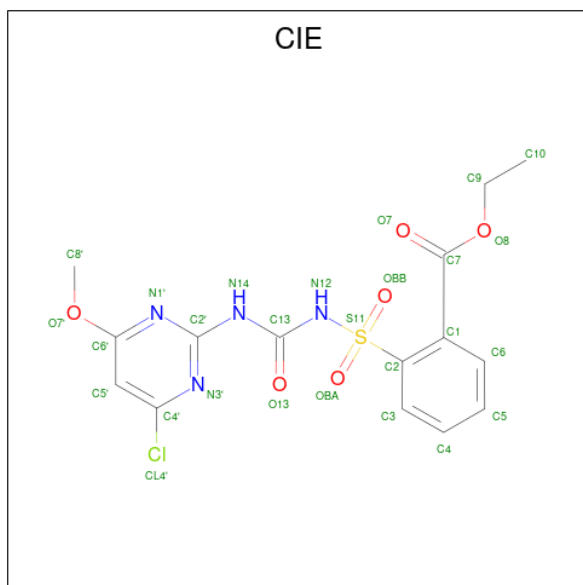
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mg	0	0
			3	3		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



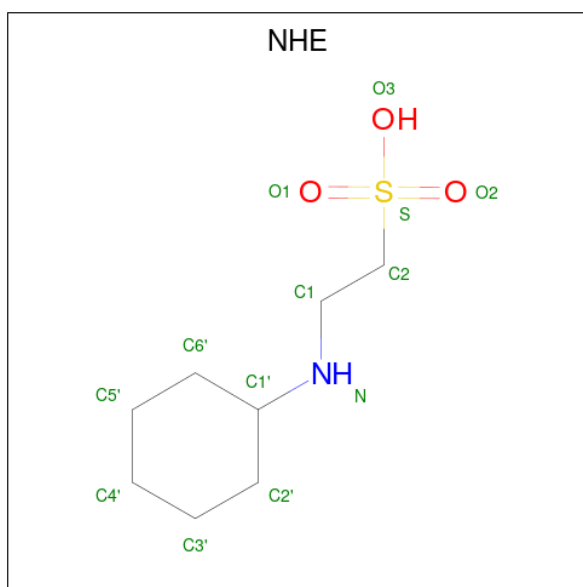
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is 2-[[[(4-CHLORO-6-METHOXY-2-PYRIMIDINYL)AMINO]CARBONYL]AMINO]SULFONYL]BENZOIC ACID ETHYL ESTER (three-letter code: CIE) (formula:  $C_{15}H_{15}ClN_4O_6S$ ).



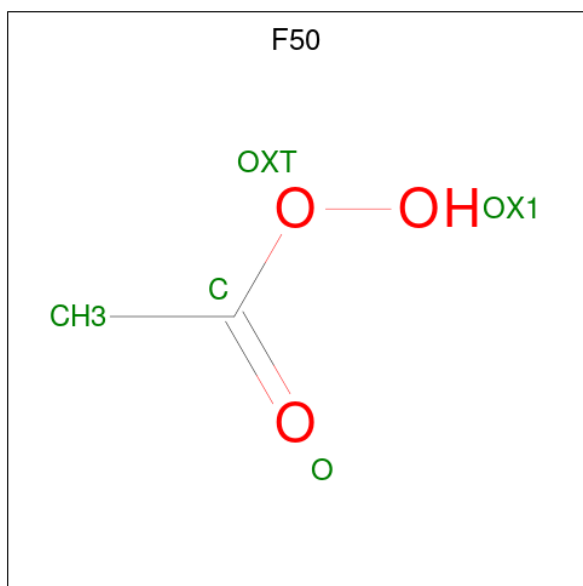
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	0
			27	15	1	4	6	1	0

- Molecule 5 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula:  $C_8H_{17}NO_3S$ ).



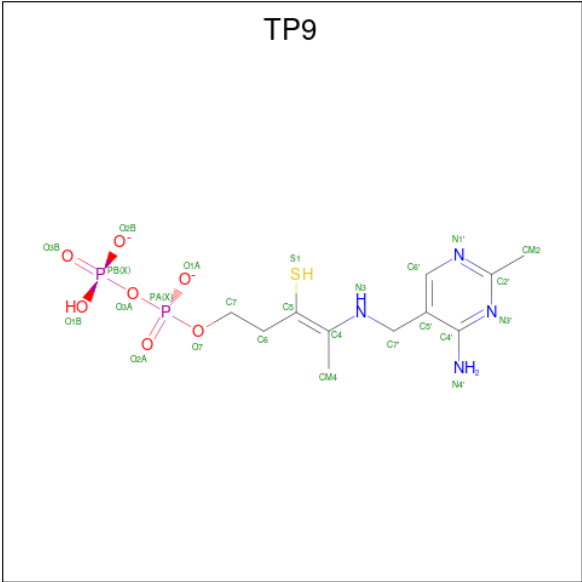
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 6 is ETHANEPEROXOIC ACID (three-letter code: F50) (formula:  $C_2H_4O_3$ ).



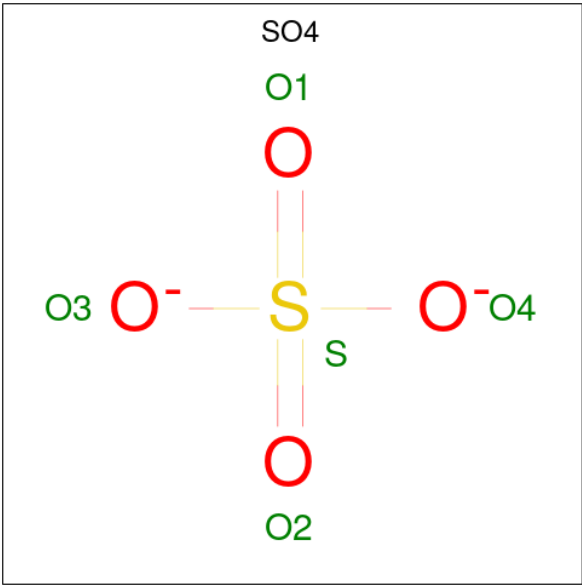
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			5	2	3		

- Molecule 7 is (3Z)-4-[[[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]AMINO}-3-MERCAPTOPENT-3-EN-1-YL TRIHYDROGEN DIPHOSPHATE (three-letter code: TP9) (formula:  $C_{11}H_{18}N_4O_7P_2S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
7	A	1	Total	C	N	O	P	S	0	1
			25	11	4	7	2	1		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

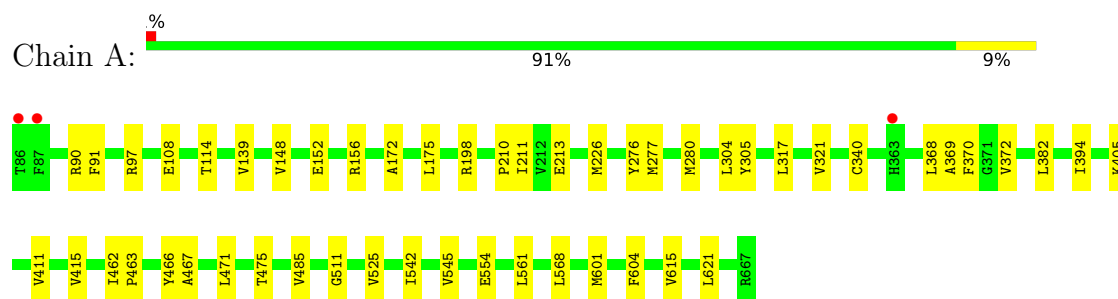


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Acetolactate synthase, chloroplastic



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.48Å 178.48Å 184.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.62 – 3.11 49.62 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.62-3.11) 99.8 (49.62-3.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.176 , 0.205 0.175 , 0.204	Depositor DCC
$R_{free}$ test set	1996 reflections (6.30%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.1	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4604	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CIE, SO4, CSD, F50, TP9, FAD, NHE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.24	0/4555	0.41	0/6182

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4468	0	4464	27	0
2	A	3	0	0	0	0
3	A	53	0	30	1	0
4	A	27	0	15	0	0
5	A	13	0	17	1	0
6	A	5	0	4	0	0
7	A	25	0	17	2	0
8	A	10	0	0	0	0
All	All	4604	0	4547	29	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (29) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ILE:HG12	1:A:411:VAL:HB	1.79	0.64
1:A:463:PRO:HG2	1:A:466:TYR:HB3	1.90	0.53
1:A:198:ARG:HG2	1:A:226:MET:HE1	1.90	0.53
1:A:601:MET:HA	1:A:604:PHE:HD2	1.76	0.51
1:A:304:LEU:HD23	1:A:368:LEU:HB2	1.95	0.49
1:A:276:TYR:N	5:A:704:NHE:O3	2.37	0.49
1:A:382:LEU:O	1:A:405:LYS:NZ	2.44	0.49
1:A:90:ARG:NH1	1:A:108:GLU:OE2	2.46	0.48
1:A:568:LEU:HD22	7:A:706[A]:TP9:H61	1.96	0.48
1:A:305:TYR:HB3	1:A:369:ALA:HA	1.95	0.48
1:A:91:PHE:CG	1:A:97:ARG:HD3	2.49	0.47
1:A:485:VAL:HG21	1:A:511:GLY:C	2.36	0.46
1:A:139:VAL:HG13	1:A:554:GLU:HG3	1.98	0.45
1:A:152:GLU:O	1:A:156:ARG:HG3	2.17	0.45
1:A:467:ALA:HA	1:A:621:LEU:HD21	1.98	0.45
3:A:702:FAD:H9	3:A:702:FAD:H1'1	1.74	0.44
1:A:277:MET:HA	1:A:280:MET:HG3	2.00	0.44
1:A:305:TYR:CE2	1:A:372:VAL:HG21	2.53	0.44
7:A:706[A]:TP9:H61	7:A:706[A]:TP9:HM41	1.70	0.44
1:A:370:PHE:HB3	1:A:415:VAL:HG21	2.00	0.43
1:A:542:ILE:HA	1:A:545:VAL:HB	2.00	0.43
1:A:210:PRO:HB2	1:A:213:GLU:HB3	2.00	0.43
1:A:148:VAL:HB	1:A:175:LEU:HD22	2.02	0.42
1:A:172:ALA:HB1	1:A:211:ILE:HG12	2.02	0.42
1:A:462:ILE:HD11	1:A:615:VAL:HG22	2.02	0.42
1:A:317:LEU:O	1:A:321:VAL:HG23	2.20	0.41
1:A:114:THR:HG21	1:A:525:VAL:HG11	2.03	0.41
1:A:471:LEU:HD22	1:A:561:LEU:HD22	2.03	0.40
1:A:471:LEU:O	1:A:475:THR:OG1	2.29	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	580/582 (100%)	569 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	479/478 (100%)	479 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	CSD	A	340	1	3,7,8	1.07	0	1,8,10	7.44	1 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	A	340	1	-	0/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	CSD	OD1-SG-CB	7.44	119.69	105.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
8	SO4	A	709	-	4,4,4	0.14	0	6,6,6	0.06	0
4	CIE	A	703	-	28,28,28	5.88	12 (42%)	38,39,39	2.96	10 (26%)
5	NHE	A	704	-	13,13,13	1.32	3 (23%)	16,17,17	1.92	5 (31%)
8	SO4	A	710	-	4,4,4	0.15	0	6,6,6	0.05	0
6	F50	A	705	-	3,4,4	1.13	0	3,4,4	3.51	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FAD	A	702	-	51,58,58	2.25	11 (21%)	60,89,89	1.52	11 (18%)
7	TP9	A	706[A]	2	21,25,25	2.63	3 (14%)	28,36,36	1.75	8 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIE	A	703	-	-	9/24/24/24	0/2/2/2
5	NHE	A	704	-	-	3/7/15/15	0/1/1/1
6	F50	A	705	-	-	0/0/2/2	-
3	FAD	A	702	-	-	14/30/50/50	0/6/6/6
7	TP9	A	706[A]	2	-	4/17/22/22	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	CIE	OBA-S11	19.90	1.66	1.43
4	A	703	CIE	OBBS11	19.49	1.65	1.43
7	A	706[A]	TP9	C4-N3	10.00	1.45	1.32
3	A	702	FAD	C10-N1	8.24	1.43	1.33
4	A	703	CIE	C2'-N14	7.24	1.48	1.38
3	A	702	FAD	C4X-C4	6.31	1.52	1.41
3	A	702	FAD	C1'-N10	-6.20	1.41	1.48
4	A	703	CIE	C2-S11	5.44	1.85	1.77
4	A	703	CIE	S11-N12	4.93	1.74	1.64
7	A	706[A]	TP9	C4'-N4'	4.59	1.45	1.34
3	A	702	FAD	C4X-N5	4.49	1.39	1.33
4	A	703	CIE	C13-N12	4.32	1.49	1.39
3	A	702	FAD	C2B-C1B	-4.27	1.47	1.53
4	A	703	CIE	C13-N14	4.18	1.46	1.37
4	A	703	CIE	O8-C7	3.25	1.41	1.33
3	A	702	FAD	O4B-C1B	3.19	1.45	1.41
3	A	702	FAD	C4-N3	3.09	1.38	1.33
4	A	703	CIE	O13-C13	-3.06	1.17	1.23
5	A	704	NHE	C2-S	3.05	1.81	1.77
4	A	703	CIE	O7'-C6'	2.81	1.39	1.35
3	A	702	FAD	O3'-C3'	-2.72	1.36	1.43
3	A	702	FAD	C2-N1	2.49	1.43	1.38
4	A	703	CIE	C4'-CL4'	2.33	1.79	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	FAD	C2'-C3'	2.32	1.57	1.53
4	A	703	CIE	C1-C7	2.28	1.55	1.50
5	A	704	NHE	O1-S	2.20	1.51	1.45
5	A	704	NHE	O2-S	2.18	1.51	1.45
7	A	706[A]	TP9	CM4-C4	2.08	1.53	1.49
3	A	702	FAD	C2B-C3B	-2.08	1.47	1.53

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	CIE	OBB-S11-OBA	-8.91	108.60	119.55
4	A	703	CIE	C4'-N3'-C2'	7.82	121.08	114.69
3	A	702	FAD	C2-N3-C4	6.19	120.36	115.14
4	A	703	CIE	C2'-N14-C13	-5.79	124.22	130.40
4	A	703	CIE	C5'-C4'-N3'	-5.67	119.28	125.50
4	A	703	CIE	C2'-N1'-C6'	5.04	120.91	114.99
4	A	703	CIE	C2-S11-N12	5.03	111.99	106.06
6	A	705	F50	OXT-C-CH3	4.88	120.08	111.09
4	A	703	CIE	C5'-C6'-N1'	-4.44	118.89	124.08
3	A	702	FAD	N3A-C2A-N1A	-4.05	122.35	128.68
5	A	704	NHE	O3-S-O1	-4.04	101.39	111.27
7	A	706[A]	TP9	C7'-N3-C4	-3.78	120.77	125.97
5	A	704	NHE	O1-S-C2	3.73	111.41	106.92
5	A	704	NHE	O3-S-C2	3.36	111.19	105.77
6	A	705	F50	OXT-C-O	-3.35	120.10	124.14
4	A	703	CIE	O8-C7-C1	3.15	118.44	112.21
7	A	706[A]	TP9	C5'-C6'-N1'	-3.09	118.66	123.82
7	A	706[A]	TP9	C6'-N1'-C2'	3.09	121.23	115.96
7	A	706[A]	TP9	PA-O3A-PB	-3.05	122.34	132.83
4	A	703	CIE	N3'-C2'-N1'	-2.98	121.51	126.23
3	A	702	FAD	C4A-C5A-N7A	-2.94	106.33	109.40
3	A	702	FAD	C4-C4X-N5	2.94	121.95	118.60
3	A	702	FAD	C9A-N10-C10	-2.74	118.32	121.91
4	A	703	CIE	C4'-C5'-C6'	2.72	118.32	114.70
5	A	704	NHE	O2-S-C2	2.69	110.16	106.92
3	A	702	FAD	C3B-C2B-C1B	2.67	104.99	100.98
3	A	702	FAD	C1'-N10-C9A	2.57	120.31	118.29
5	A	704	NHE	C1-N-C1'	-2.54	109.15	114.14
3	A	702	FAD	C10-C4X-N5	-2.43	119.58	121.26
7	A	706[A]	TP9	N4'-C4'-N3'	2.34	120.34	117.03
7	A	706[A]	TP9	N1'-C2'-N3'	-2.31	121.57	125.54
7	A	706[A]	TP9	C6'-C5'-C4'	2.27	118.81	115.72

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	706[A]	TP9	CM4-C4-N3	2.25	120.52	118.00
3	A	702	FAD	C10-C4X-C4	-2.24	118.47	119.95
3	A	702	FAD	C4X-C4-N3	-2.14	120.50	123.43
3	A	702	FAD	P-O3P-PA	-2.10	125.62	132.83

There are no chirality outliers.

All (30) torsion outliers are listed below:

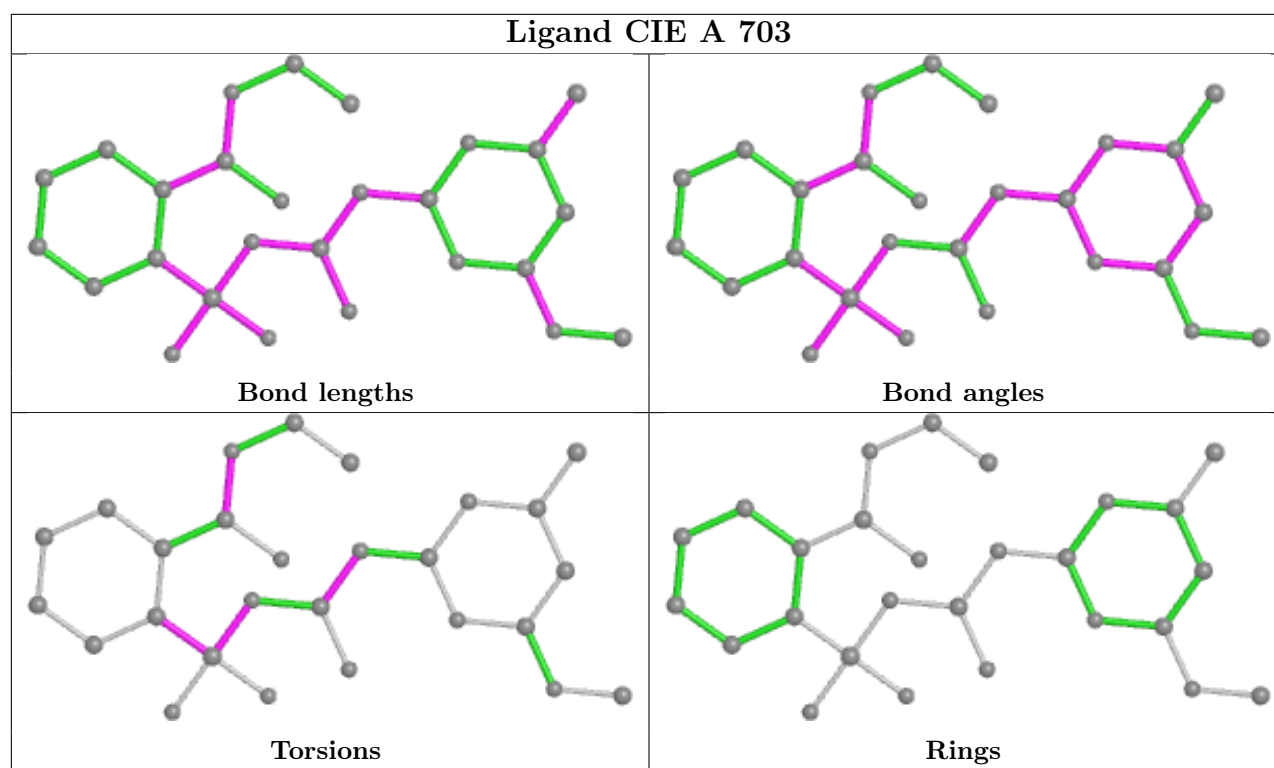
Mol	Chain	Res	Type	Atoms
3	A	702	FAD	C2'-C1'-N10-C9A
3	A	702	FAD	C1'-C2'-C3'-C4'
3	A	702	FAD	C3'-C4'-C5'-O5'
3	A	702	FAD	O4'-C4'-C5'-O5'
4	A	703	CIE	N12-C13-N14-C2'
5	A	704	NHE	C1-C2-S-O1
7	A	706[A]	TP9	C4-C5-C6-C7
4	A	703	CIE	C1-C7-O8-C9
4	A	703	CIE	O7-C7-O8-C9
4	A	703	CIE	C13-N12-S11-OBA
3	A	702	FAD	O3'-C3'-C4'-C5'
5	A	704	NHE	C1-C2-S-O3
3	A	702	FAD	C2'-C3'-C4'-C5'
3	A	702	FAD	O2'-C2'-C3'-C4'
4	A	703	CIE	C3-C2-S11-OB
3	A	702	FAD	C2'-C3'-C4'-O4'
4	A	703	CIE	C1-C2-S11-OB
4	A	703	CIE	C1-C2-S11-N12
7	A	706[A]	TP9	PB-O3A-PA-O7
3	A	702	FAD	O2'-C2'-C3'-O3'
5	A	704	NHE	C1-C2-S-O2
3	A	702	FAD	N10-C1'-C2'-O2'
3	A	702	FAD	O3'-C3'-C4'-O4'
4	A	703	CIE	O13-C13-N14-C2'
4	A	703	CIE	C3-C2-S11-N12
7	A	706[A]	TP9	C5-C6-C7-O7
3	A	702	FAD	O4B-C4B-C5B-O5B
7	A	706[A]	TP9	C7-O7-PA-O2A
3	A	702	FAD	C1'-C2'-C3'-O3'
3	A	702	FAD	C4B-C5B-O5B-PA

There are no ring outliers.

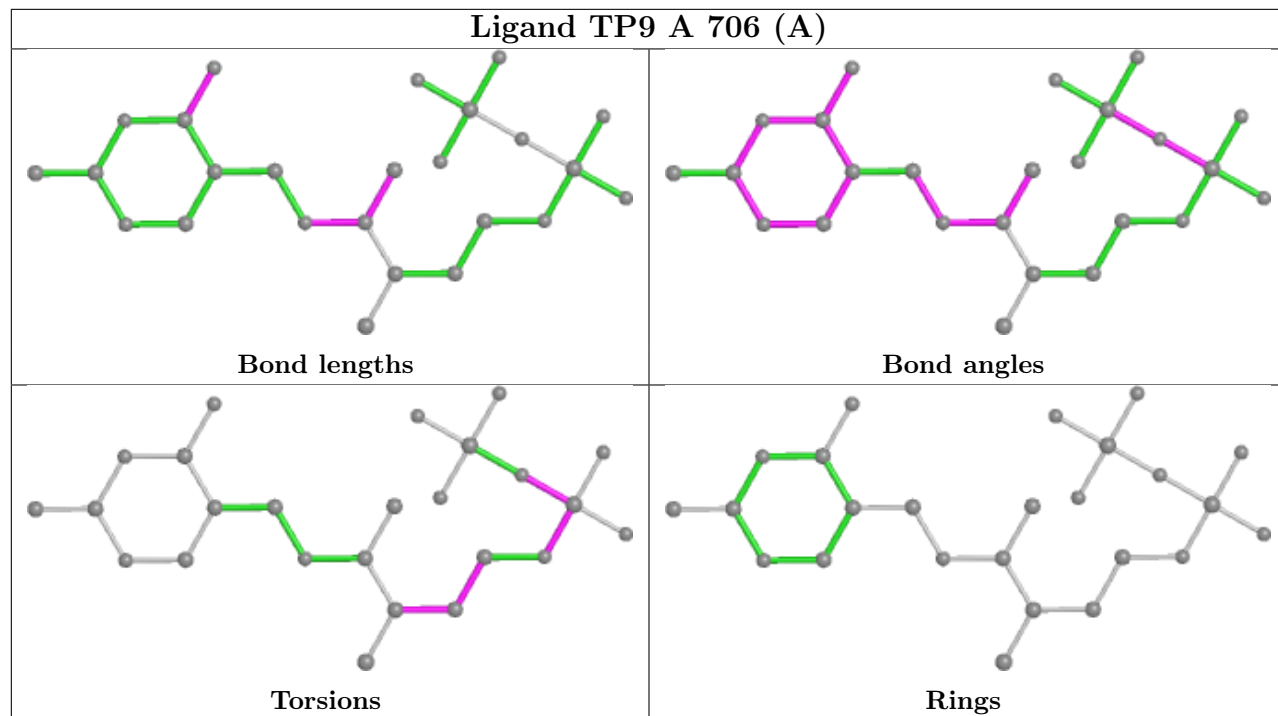
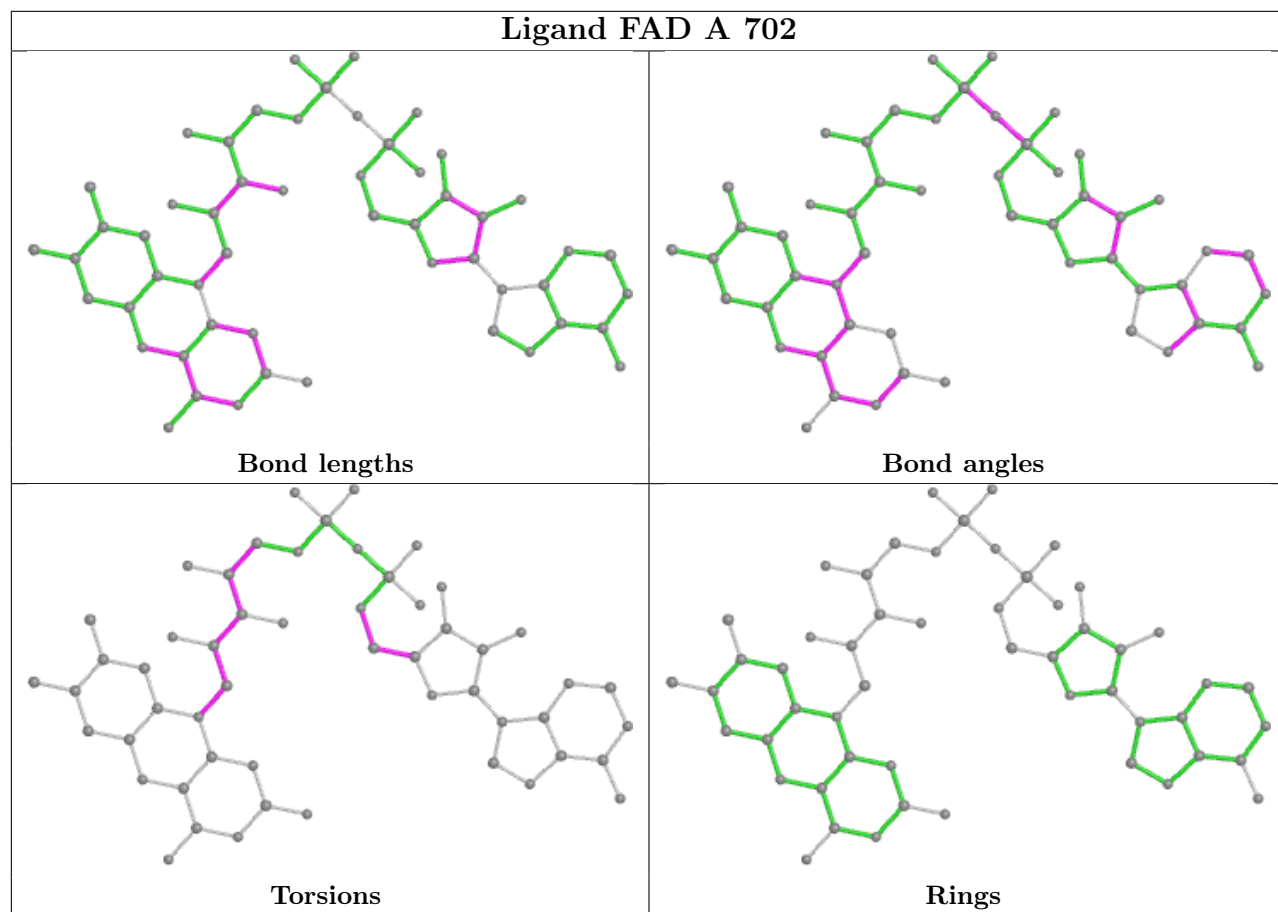
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	704	NHE	1	0
3	A	702	FAD	1	0
7	A	706[A]	TP9	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	581/582 (99%)	-0.16	3 (0%) <a href="#">91</a> <a href="#">82</a>	54, 78, 108, 132	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	THR	2.2
1	A	87	PHE	2.0
1	A	363	HIS	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSD	A	340	8/9	0.87	0.19	59,90,97,103	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

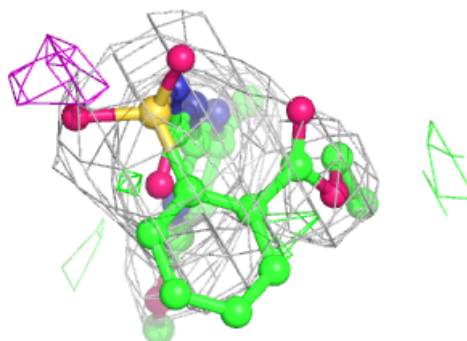
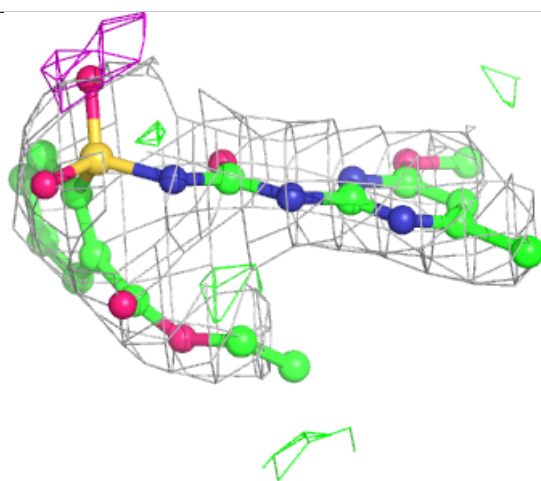
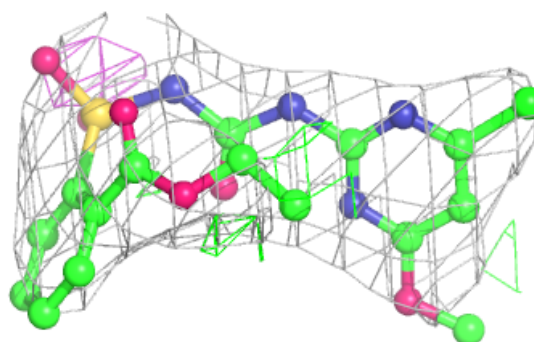
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	708	1/1	0.79	0.28	105,105,105,105	1
8	SO4	A	710	5/5	0.81	0.49	108,111,137,146	5
8	SO4	A	709	5/5	0.84	0.29	83,94,105,123	5
2	MG	A	701	1/1	0.84	0.29	69,69,69,69	0
6	F50	A	705	5/5	0.88	0.30	74,78,88,89	5
2	MG	A	707	1/1	0.94	0.17	64,64,64,64	1
5	NHE	A	704	13/13	0.95	0.18	66,90,103,106	0
4	CIE	A	703	27/27	0.96	0.18	68,89,106,112	27
3	FAD	A	702	53/53	0.97	0.17	45,72,82,92	0
7	TP9	A	706[A]	25/25	0.98	0.26	65,75,84,100	25

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

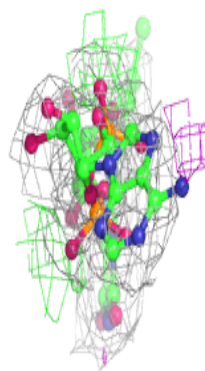
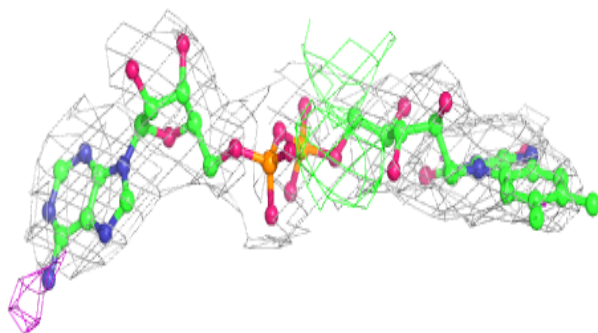
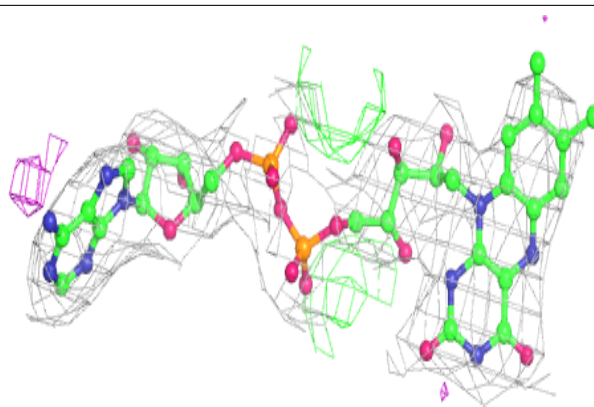
#### Electron density around CIE A 703:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

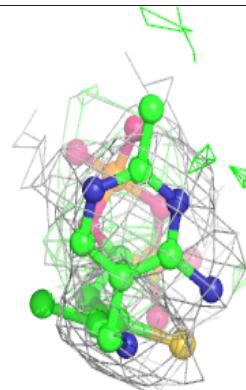
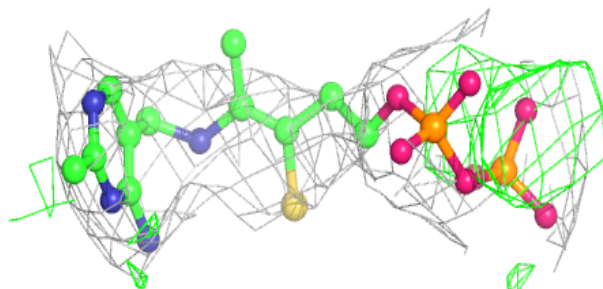
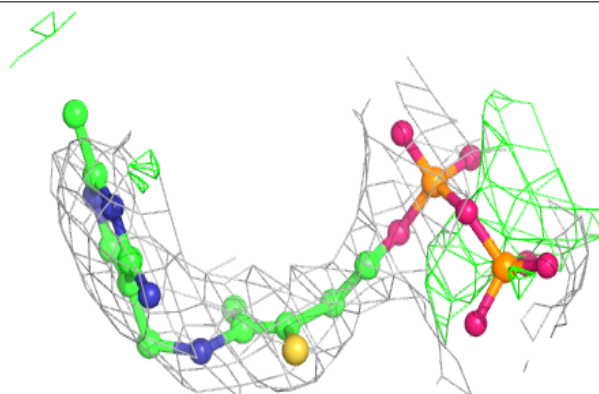


**Electron density around FAD A 702:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around TP9 A 706 (A):**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.